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Band structure and magnetic properties of cubic crystals $In_xGa_{1-x}N$: Ab initio calculations*

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Зонная структура и магнитные свойства кубических кристаллов $In_xGa_{1-x}N$: Ab initio расчёты***

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Band structure of solid solutions $In_xGa_{1-x}N$ with sphalerite structure and with considerable percentage of indium (x = 0,25; 0,5; 0,6; 0,7; 0,75; 0,9; 0,95; 0,97; 0,99; 1,0) is calculated using the density-functional theory (DFT) and the cluster version of the local coherent potential method within the frame of the multiple scattering theory. The electron structure of the ternary solutions of $In_xGa_{1-x}N$ in sphalerite crystallographic modification is compared; the interpretation of their features is given. The concentration dependence on the energy gap for the entire variation range of the indium content in the solution is obtained. The spin polarization effect of the states of In, Ga, and N for the alloys with the considerable percentage of In, as well as the transition of the ternary solutions of $In_{0.75}Ga_{0.25}N$ into the of magnetic semiconductor state is found out. The magnetic moments of In, Ga, and N atoms, and the saturation magnetization in $In_xGa_{1-x}N$ semiconductor system are determined.

Keywords: band structure, magnetic moment, valence band, band gap, density of electronic states.

Зонная структура твёрдых растворов $In_xGa_{1-x}N$со сфалеритной структурой и большим содержанием индия (*x* = 0,25; 0,5; 0,6; 0,7; 0,75; 0,9; 0,95; 0,97; 0,99; 1,0) рассчитана методами теории функционала плотности (DFT) и кластерной версии локального когерентного потенциала, в рамках теории многократного рассеяния. Проведено сравнение электронной структуры тройных растворов $In_xGa_{1-x}N$сфалеритной кристаллографической модификации, дана интерпретация их особенностей. Получена концентрационная зависимость ширины запрещённой полосы для всего диапазона изменения содержания индия в растворе. Обнаружен эффект спиновой поляризации состояний In, Ga и N для растворов с большим молярным содержанием In и переход тройных систем $In_{0.75}Ga_{0.25}N$в состояние магнитного полупроводника. Определены магнитные моменты на атомах In, Ga и N и намагниченность насыщения полупроводниковой системы $In_xGa_{1-x}N$.

Ключевые слова: зонная структура, магнитный момент, валентная зона, ширина запрещённой полосы, плотность электронных состояний.

Introduction. The semiconductor solid solutions $In_xGa_{1-x}N$ are the most promising materials for optoelectronics to obtain the blue and green light-emitting diodes which are used for high-density optical storage of information and high-power devices, for blue lasers for instance. The extraordinary property of these materials is the ability to operate over a wide temperature range and the insensitivity to X-ray irradiation [1, 2]. By varying of the indium percentage one can manage the value of the energy gap in the range from 1.92 eV (c-InN) [3] upto 3.2 eV (c-GaN) [3] that gives the opportunity to use these materials in various parts of spectrum [4, 5]. For the far ultraviolet region (240-300 пм) the semiconductor materials based on $In_xGa_{1-x}N$ (0,5< x < 1) crystals are of high interest.

The alloys $In_xGa_{1-x}N$ with the high percentage of indium are studied not sufficiently in comparison with other nitrides of III group elements because of the difficulties connected with the growing of such crystals [6]. On the top of c-GaN buffer lay it is possible to grow up a film of alloy In-Ga-N of high quality with cubic structure [3, 7] using the method of gas-source molecular beam epitaxy. The theoretical investigation of these alloys $In_xGa_{1-x}N$ ($0 < x \le 0,75$) were performed using the densi-

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ty-functional theory (DFT) in the local density approximation (LDA) [2, 4]. The structural, termodynamical properties, and the composition dependence of bowing parameter of the calculated band gap have been determined. It was shown that this bowing parameter was due to structure effect that is to the structure induced disordering of the bond lengths, and depends on the fraction of indium. Nevertheless the mechanism of the influence of indium atoms on the energy gap in $In_xGa_{1-x}N$ alloy has not been elucidated, for 0.75 <x< 1 especially.

The heightened interest to the search of new so called magnetic semiconductors (MS) is due to their key role for creation of new devices of spintronics [8, 9]. The most traditional way is to admix magnetic d-atoms, Mn-atoms for example, into the semiconductor matrix GaN. It leads to the rise of special magnetic properties particular for ferromagnetic materials with the high Curie temperature [10]. The admixture of Ga-atoms into the epitaxial films of GaN as was shown by magnetometry [11] results in the origin of the giant magnetic momentum at gadolinium atom. The alloyed layers of GaN:Gd demonstrate the ferromagnetism with the temperature of transition into magnetic order state higher than room temperature. Because of this the system GaN:Me looks promising for spin electronics.

Quite other way of creation of dilute magnetic materials is possible using effect of spin polarization by admixture of non-magnetic atoms into the non-magnetic matrix. For instance for BeO: (B, C, N) system it was shown [12], that by the partial substitution oxygen atoms in BeO by atoms boron, carbon or nitrogen the spin polarization of ($2p_\uparrow - 2p_\downarrow$)-states occurs, and the system BeO : X becomes to be magnetic semiconductor (BeO : B) or magnetic semimetal (BeO : C, N). The ternary systems $In_xGa_{1-x}N$ and the binary basic systems GaN and InN are usually considered as non-magnetic semiconductors. Because of this there are no publications with spin-polarized calculations of zone structure of such materials.

In the present work the zone structure, forbidden energy band bowing and magnetic properties of wide band semiconductors $In_xGa_{1-x}N$ with the great percentage of indium using the methods of functional density theory (spin-polarized version) and the cluster version of local coherent (spin-restricted version) were investigated.

Models and methods. The crystallographic structure of the ternary system $In_xGa_{1-x}N$ is of cubic sphalerite-type, its space group is $\bar{F}43m$. The coordination polyhedral (CP) of the atoms In and Ga are tetrahedral $\left[MeN_4\right]$. Interatomic distances are supposed to be: $Ga - N = In - N = a\sqrt{3}/4$, where a is the lattice parameter, which was determined according to Vegard's law.

Zone calculations of electron structure of nitrides $In_xGa_{1-x}N$ (x = 0; 0,25; 0,5; 0,6; 0,7; 0,75; 0,9; 0,95; 0,97; 0,99; 1,0) were performed with the spin-polarized full-potential method of pseudopotential (program package Quantum-Espresso [13]) using the theory of the functional density (DFT) developed by Kohn and Sham [14] . In this theory the total energy of the unite cell is the sum of the one-electron energy, Hartree energy, exchange-correlation energy, and electrostatic Ewald energy, and the non-local exchange-correlation functional in the form Perdew-Burke-Ernzerhof (PBE) [15].

The following electron configurations of atoms have been used: In — [Kr]$5s^25p^14d^{10}$, N — [He]$2s^22p^3$, Ga — [Ar]$4s^24p^13d^{10}$. For atoms In, Ga and N the electrons in the states $5s^25p^14d^{10}$, $4s^24p^13d^{10}$, and $2s^22p^3$ were attributed to valence ones correspondingly, whereas the electrons of completely occupied shells [Kr], [Ar], and [He] were considered as core-electrons. The influence of core-electrons was taken into account by using ultrasoft pseudopotentials for indium atom (code Dal Corso [13]) whereas for gallium and nitrogen atoms the code Vanderbilt (versions 735 и 734) [15] was used.

The plane waves set was "cut off" at the energy 20 Ry that provided the convergence of the total energy of the cell in our self-consistent calculations not worse than 0,001 Ry. The density of electron states was calculated using the rectangular grid of points of dimensions 4x4x4, spaced evenly throughout the Brillouin zone (Monkhhorst-Pack grid).

The electron densities $\rho(r)$ in the real space and the partial densities of electron states (DOS) in valence and conduction bands were calculated separately for every spin projection similar way as in [12]. It gave us the possibility to determine connected with spin magnetic moment at every atom.

To investigate the electron structure of the system Ga-In-N with the great fraction of indium the local coherent potential ab initio method in the frame of multiple scattering theory was used. This method was developed in our group and applied for many systems, for Ti-Al-C system for instance [16]. The approximation of virtual crystal is quite effective approach for the system under investigation with the percentage of an element of any possible value. The muffin-tin approximation for crystal potential was used. The latter was the sum of Coulomb, exchange (Slater's version) and Madelung contributions. The local

partial densities for every component of alloys was calculated for cluster of 250 atoms of the system In-Ga-N according to expression

$$n^{In}{}_1(E) = \frac{-\sqrt{E}}{\pi} \int_0^{Rws} \{ rR_l^{In}(r,E) \}^2 dr \frac{Im Tr T_{lm,lm}^{00,In}}{Im t_l^{0In}}$$

where l is the orbital quantum number, $R_l(r,E)$ are the radial wave functions, T is a matrix element of the scattering operator, and index 0 shows the centre at which the atom In is placed.

Results and discussion.

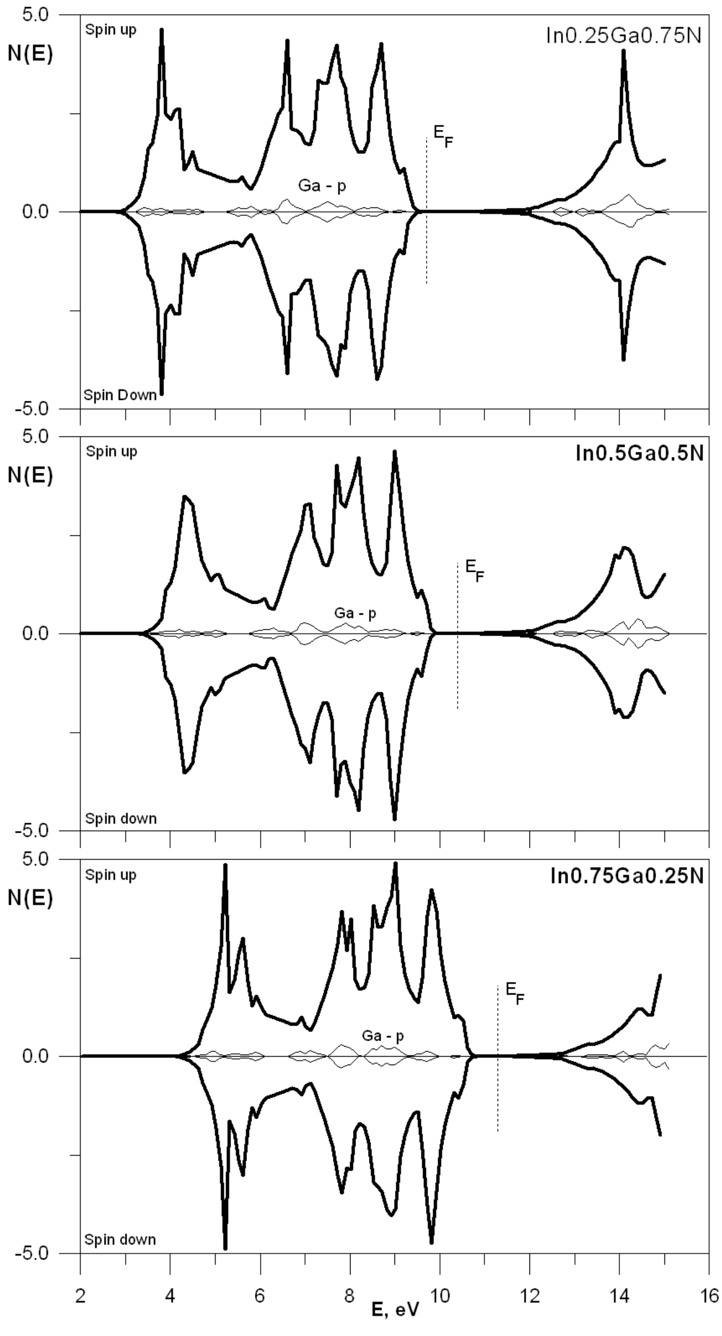


Fig. 1 – Total densities of states for $In_xGa_{1-x}N$ (x = 0,25; 0,5; 0,75).

Band structure and magnetic properties. The band structure of cubic $In_xGa_{1-x}N$ system changes significantly as the molar fraction x of indium increases. It concerns both occupied valence and unoccupied conduction bands. In Fig. 1 the total

electron densities of states for both spin orientations (TDOS) for solid solutions $In_xGa_{1-x}N$ (x = 0.25; 0.5; 0.75) are shown. One can see the features in comparison to TDOS of the c-GaN (Fig.2).

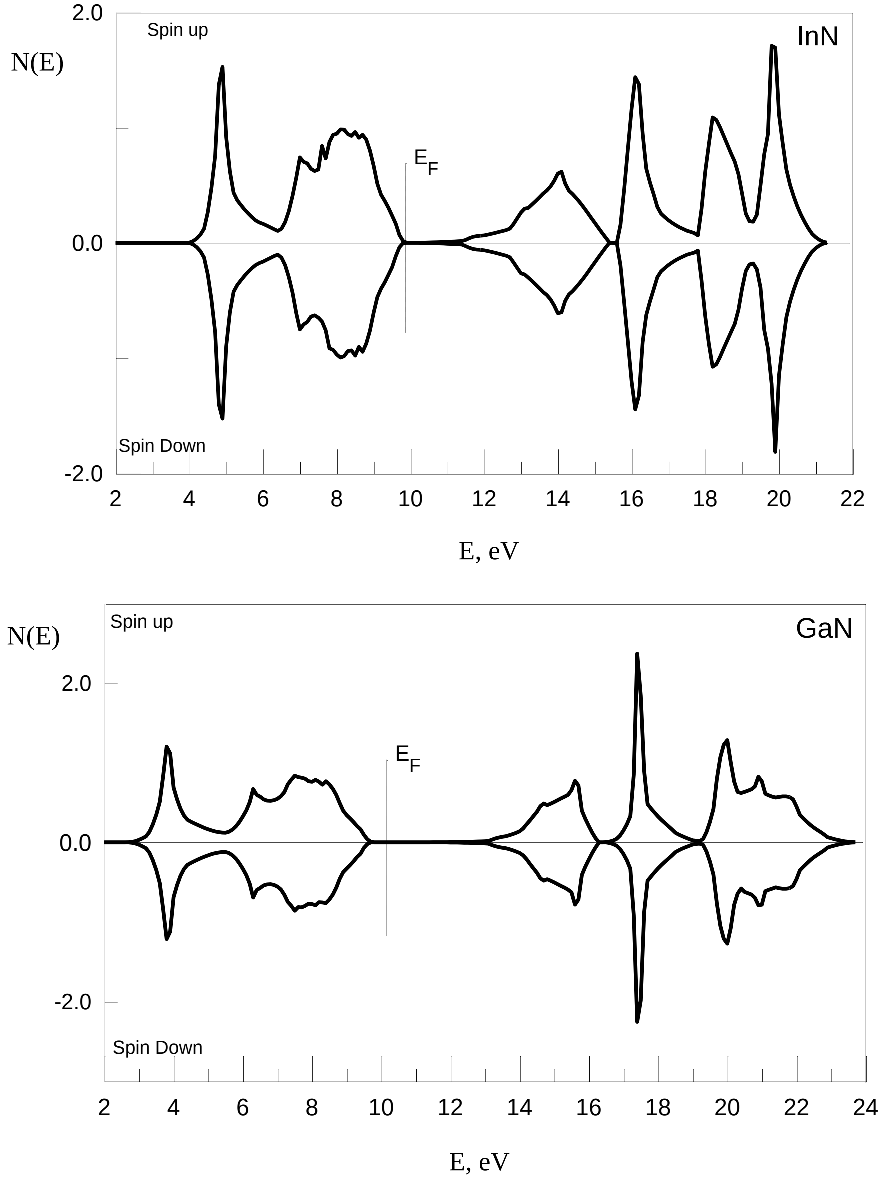


Fig. 2 - Total densities of states for InN and GaN (x = 0,25; 0,5; 0,75).

The most significant changes of electron structure happen for $In_{0.25}Ga_{0.75}N$ and $In_{0.75}Ga_{0.25}N$. These changes are connected with the interaction In4d- and Ga3d-obitals with 2p-obitals of nitrogen which results in the changes of the electronic and magnetic properties of the system under consideration.

The valence band (VB) is formed by states essentially of 2p-electrons of nitrogen atoms with the admixture of s- and *p*-states of Ga and In and distinguishes the high energy localization of In5s- (3,8 eV), In5p- and Ga4p- (6,6 eV and 7,7 eV), and 2p-states of nitrogen (8.7 eV). The corresponding maxima of TDOS for both spin orientations can one see for all alloys. At the same time for $In_{0.25}Ga_{0.75}N$ there are some band gaps which can be seen on the curves of local densities of electron states for both spin subsystems $N_{\uparrow}(E)$ и $N_{\downarrow}(E)$ of indium, gallium and nitrogen, as well as appearance of unoccupied states of In5s- and Ga4s-electrons at 0,6 eV from Fermi level (Fig.3) which can be treated as acceptor level.

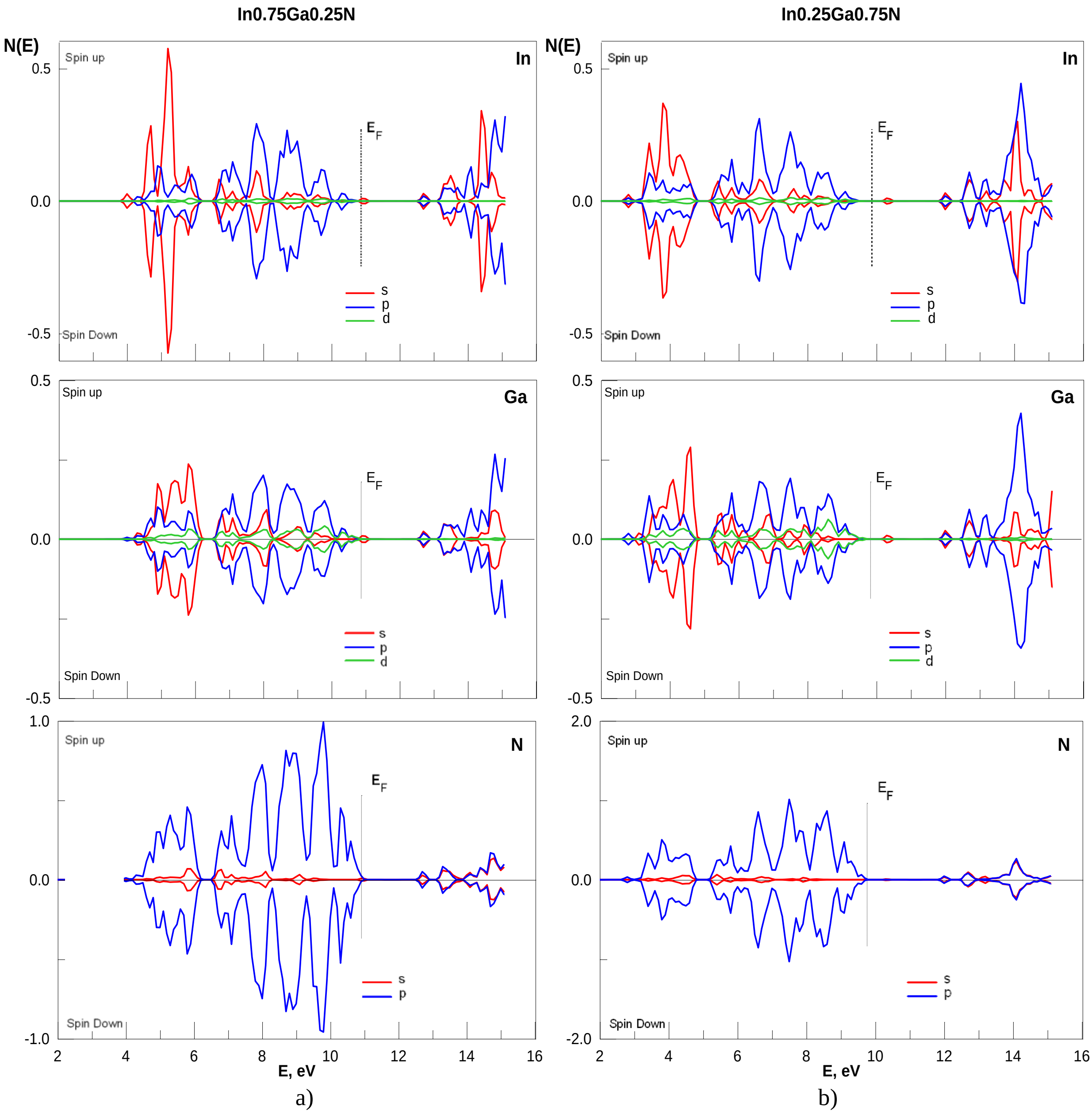


Fig. 3. Partial atomic densities of states for $In_{0.25}Ga_{0.75}N$ (a) and $In_{0.75}Ga_{0.25}N$ (b)

At significant molar fraction of indium (for example x = 0,75) the bands of occupied and free electron states shift to the greater energies by more than 1,0 eV in comparison to $In_{0.25}Ga_{0.75}N$. The energy gap E_g of $In_{0.75}Ga_{0.25}N$ decreases by 0.5 eV and is equal to 1,9 eV.

By integration of electron local partial densities for every spin projection for the systems $In_xGa_{1-x}N$ (x = 0; 0,25; 0,5; 0,75; 1,0) provides us the local partial charges of atoms and the possibility to determine the spin magnetic moments at every kind of atoms (Table1). It was ascertained that the ternary system under investigation displayed rather small magnetic moment at atoms Ga, In, and N, which value increases in the row $In_{0.25}Ga_{0.75}N \rightarrow In_{0.5}Ga_{0.5}N \rightarrow In_{0.75}Ga_{0.25}N$. The greatest spin splitting takes place for 4p-shell of gallium atom, that causes the appearance of magnetic moment at Ga atom 0,009μ_B, whereas the magnetic moments at atoms of matrix indium and nitrogen in $In_{0.75}Ga_{0.25}N$ are equal to 0,008 μ_B. In this system, when x = 0.75 the Ga atoms can be considered as admixture atoms.

Table 1.

The structural parameters, magnetic moments at atoms and absolute magnetization Ms (at T = 0K) in the systems $In_xGa_{1-x}N$

	Lattice parameter, Å	Cell volume, (a.u.)^3	Magnetic moments, μ_B			M_S, μ_B/cell
			In	Ga	N	
c-GaN	4,500	153,73	-	0,009	- 0,009	0,05
$In_{0.25}Ga_{0.75}N$	4,655	680,69	0,006	0,007	0,007	0,17
$In_{0.5}Ga_{0.5}N$	4,740	718,67	0,007	0,008	0,008	0,18
$In_{0.75}Ga_{0.25}N$	4,770	732,40	0,009	0,009	- 0,008	0,19
c-InN	4,980	208,36	0,010	-	0,010	0,06

It is worth to mention that in binary compounds GaN and InN there are magnetic moments. For instance for c-GaN are there magnetic moments at atoms Ga (0,009 μ_B) and N (- 0,009 μ_B), but it does not lead to the ferromagnetism of this compound because two sublattices are magnetized antiparallel ways. These results agree with the molecular Weiss' theory, according to which the magnetization of every sublattice $M^{A,B}$ is determined by the sum of average statistical magnetization of separate ions $<<\mu^{A,B}>>$ by analogy with [17] $M^{A,B}=\frac{N}{2}<<\mu^{A,B}>>$, where N - the number of atoms and $<<\mu^{A,B}>>$ - a quantum-mechanical average magnetic moment of the n-level.

Thus the resulting magnetization in binary and ternary systems $In_xGa_{1-x}N$ (x = 0; 0,25; 0,5; 0,75; 1,0) is the sum of the magnetization of magnetic sublattices and is determined by the set of levels E_n in common nearly the ground state. Our a*b initio* calculations of the electron structure and the total and the absolute magnetization of binary and ternary systems gave for the total magnetization the zero estimation $M=0$ but the absolute magnetizations $M_s>0$ is different from zero (Table 1). The magnetization of saturation M_s (for $T=0\,K$) of the semiconductor materials under investigation increases monotonous way with x and achieves 0,19 μ_B/cell for x = 0,75, being small for all x. It is possible to suppose that the systems GaN, InN, and $In_xGa_{1-x}N$ are in paramagnetic state. The appearance of ferromagnetic properties of GaN layers by admixture of Gd atoms was noted earlier [11], and was connected with the giant magnetic moment at the atom of gadolinium. Unfortunately the measurements of the magnetic moments at atoms of Ga and N have not been carried out.

The creation of magnetic moments at atoms of nitrogen (0,42 μ_B) was observed in BeO : N [12] by the partial substitution of oxygen atoms by nitrogen atoms. The nature of the creation of magnetic properties of nitrogen atoms in the system BeO: N the authors of paper [12] explain by the mutual energy position of the valence O2*p*-band of matrix and 2*p*-band of nitrogen atoms which is determined by the difference of orbital energies $\Delta\varepsilon$ (O2*p* – N2*p*) = -1,749 eV, that leads to the spontaneous polarization of N($2p_\uparrow - 2p_\downarrow$)-states and converts the system BeO : N into the state of magnetic semimetal (MSM). It was shown [12] that by diminishing of the difference of the orbital energies $\Delta\varepsilon$ in the system BeO : (B, C, N) the magnetic moments of admixturing atoms decrease noticeably (from 1,16 μ_B for BeO : B to 0,42 μ_B for BeO : N), magnetic moments at atoms of beryllium and oxygen as well as the total magnetization of such system decrease also.

However for the semiconductor system $In_xGa_{1-x}N$ the results of the work [12] about the role of the mutual positions of *p*-orbital energies of admixtural atoms and the atoms of non-metallic lattice cannot be used because alloying in the system $In_xGa_{1-x}N$ is performed into metallic sublattice and secondly, the energy of 2*p*-orbital of nitrogen (-11,4852 eV) [18] is situated lower than the energies of *p*-orbital In (- 4,6947 eV) [18] and Ga (- 4,9218 eV) [18] The differences of energies $\Delta\varepsilon$ of *p*-orbitals in one case are equal: for nitrogen $\Delta\varepsilon$ (Ga4*p* – N2*p*) = 6,563 eV and for indium $\Delta\varepsilon$ (In5*p* – Ga4*p*) = 0.227 eV. So for instance in the system $In_{0.75}Ga_{0.25}N$ the magnetic moment at the atom nitrogen is more than 4 times less than in system BeO:N, that can be connected with the influence of the element composition of matrix, crystallographic and electron zone structures.

The analysis of the partial charges of both spin subsystems $N_\uparrow(E)$ an $N_\downarrow(E)$ in the semiconductor alloy $In_{0.75}Ga_{0.25}N$ (Table 2) allows us to state that spontaneous spin polarization of the electron states Ga ($4p_\uparrow$ - $4p_\downarrow$)-, In($5p_\uparrow$ - $5p_\downarrow$), and N($2p_\uparrow$ - $2p_\downarrow$) give main contributions into magnetic moment when there are no external magnetic fields. The contributions into magnetization of lattice ions of the electrons of Ga4*s*-, In5*s*-, and N2*s*-orbitals turn out to be 2 times less than of their *p*-electrons. It is while to note that Ga3*d*- and In4*d* -states of the valence band electrons make no noticeable contribution into the magnetic moments at atoms of the system $In_xGa_{1-x}N$.

Table 2.

Partial charge distribution of valence electrons at atoms for the spin subsystems N↑(E) и N↓(E) in $In_{0.75}Ga_{0.25}N$

	In			Ga			N	
	s	p	d	s	p	d	s	p
n↑	0,3819	0,6840	4,9855	0,4342	0,7205	4,9967	0,7473	2,1651
n↓	0,3797	0,6790	4,9856	0,4313	0,7143	4,9967	0,7480	2,1721
(n↑- n↓)	0,0022	0,0050	-0,0001	0,0029	0,0062	0,0000	-0,0007	-0,0070
∑	0,7616	1,3631	9,9711	0,8655	1,4347	9,9934	1,4953	4,3372

The dependence $E_g(x)$.By increasing of the molar fraction of indium in the system $In_xGa_{1-x}N$ in spite of significant change of the electron energy structure both in occupied and unoccupied bands, it is possible to state that the width of the valence band conserves its value, the VB and Fermi level shift by more than 1 eV to the higher energies, and the width of forbidden energies E_g decreases from 2,4 eV (x = 0,25) to 1,9 eV (x = 0,75). The calculated composition dependence $E_g(x)$ in c-$In_xGa_{1-x}N$(x = 0; 0,25; 0,5; 0,75; 1) appears to be nonlinear one and is shown in Fig. 4, where it is compared with the experimental data [2]. One can see the good agreement of received theoretically in the present work and experimental data.

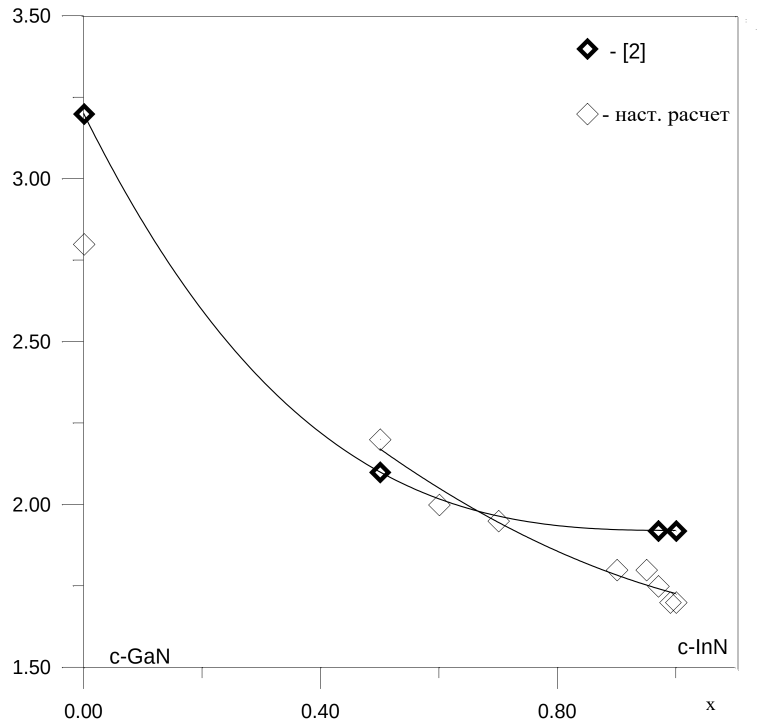


Fig. 4. Composition dependence curve $E_g(x)$ for alloys c-$In_xGa_{1-x}N$ (x = 0;0,25;0,5;0,75; 1)

The form of the composition dependence curve $E_g(x)$ for alloys c-$In_xGa_{1-x}N$ (x = 0; 0,25; 0,.5; 0,75; 1) is analogous of one found earlier [19] for the cubic alloys c-$Al_xGa_{1-x}N$ and does not contradict usual notions of physics. The value of bowing parameter at indium fraction x = 0,5is the greatest one and equals to 0.25 eV.

Interatomic interactions. Some particularities of the interatomic interaction in cubic alloysc-$In_xGa_{1-x}N$ on can observe on the maps of total electron density (ED) in the real space. For example in Fig. 5 the maps of ED are demonstrated for $In_{0.25}Ga_{0.75}N$ in the planes (110) and (001). One can see, that along the lines Ga-N and In-N the covalent type bonds prevail. The localization of ED for In-N bond is expressed explicitly that is the evidence of creation of hybridized orbitals In4*d*-N2*p* and Ga3*d*-N2*p*. The interaction of atoms of metallic sublattice is metallic one, whereas the bonds Ga-In are of directing type and are formed by In2*p*- and Ga2*p*-states in the energy range from 6.5 to 11 eV.

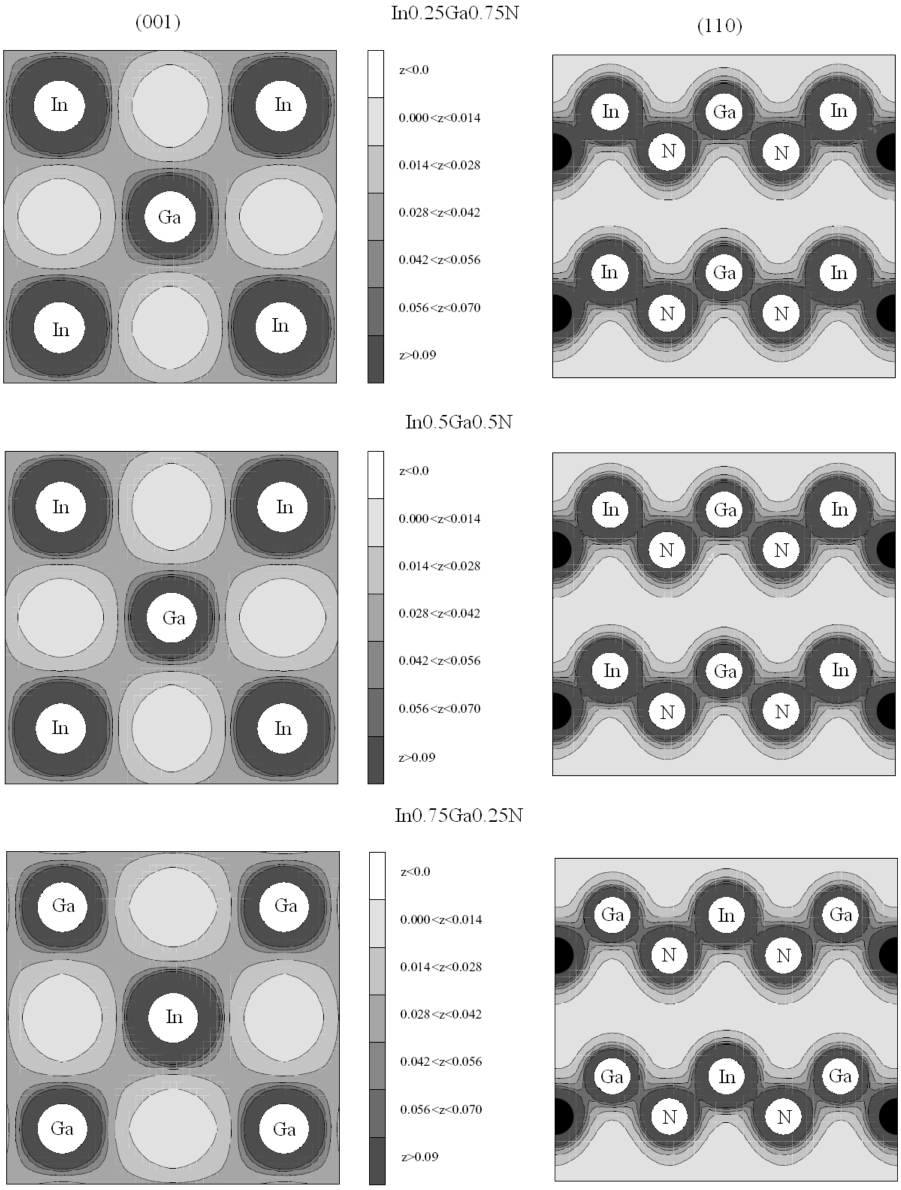


Fig. 5 – The total density maps in Ga-N and In-N (001) and (110) planes according to $In_xGa_{1-x}N$ (x = 0,25; 0,5; 0,75)

The analysis of electron energy spectra (Fig. 3a and 3b) which have the resonance character shows that the creation of localized hybridized orbitals In5*s*-N2*p* and Ga4*s*-N2p in the energy interval from 4 to 10 eV is possible.

Conclusion. With application of ab initio zone quantum-mechanical method using the density functional theory and with the cluster version of the local coherent potential approach the systematic calculations of electronic and magnetic properties of cubic alloys $In_xGa_{1-x}N$ for various molar fractions $0 \le x \le 1$ of indium were carried out.

In the row GaN→ $In_{0.25}Ga_{0.75}N$→ $In_{0.5}Ga_{0.5}N$→ $In_{0.75}Ga_{0.25}N$ we have observed: the shift of VB to the higher energies by more than 1.0 eV, the decreasing of energy gap E_g , which equals for $In_{0.99}Ga_{0.01}N$ ≈ 1,7 eV, the appearance of acceptor levels above Fermi energy due to In and Ga atoms and resonance electron states of *s*- and *p*-symmetry in unoccupied band.

The results of our calculations of partial local electron densities of states for spin subsystems $N_\uparrow(E)$ and $N_\downarrow(E)$ permit us to assert the existence of the spin polarization effect of atoms In, Ga, and N in the system $In_xGa_{1-x}N$, that transmits it into the state of magnetic semiconductor. The magnetic moments of atoms In, Ga, and N has been calculated as well as saturation magnetization of the system $In_xGa_{1-x}N$, which can be treated as the evidence of the paramagnetic state of this material. Thus, in cubic crystals $In_xGa_{1-x}N$ with the great fraction of indium the effect of spin splitting of zone Ga4(*s*-, *p*-), In 5(*s*-, *p*-), and N2*p* was observed which leads to creation of magnetic moments about $0.01\mu_B$ at atoms of both sublattices. At the same time these atomic magnetic moments In ($0{,}009\mu_B$), Ga ($0{,}009\mu_B$), and N ($-0{,}008\mu_B$) does not lead to ferromagnetism because the magnetic moments of atoms of two sublattices are antiparallel, which is in accordance with molecular theory of Weiss.

References

1. Nakamura, S. InGaN-based blue light-emitting diodes and laser diodes. Journal of Crystal Growth, 1999, vol.202, pp. 290-295.

2. Ferhat, M., Bechstedt, F. First-principles calculations of gap bowing in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys: Relation to structural and thermodynamic properties. Physical Review B, 2002, vol. 65, pp. 075213-1 -075213-8.

3. Li, J.B., et al. Cubic InGaN grown by MOCVD. MRS Internet Journal of Nitride Semiconductor Research, 1999, vol. 4S1, G3.25.

4. Krivolapchuk, V.V., Lundin, V.V., Mezdrogina, M.M. The role of inserting electrical fields in the formation of the radiation of quantum wells InGaN/GaN. Fizika Tverdogo Tela, 2005, vol. 47, no. 7, pp. 1338-1342.

5. Ferhat, M., Furthműller, J., Bechstedt, F. Gap bowing and Stokes shift in InxGa1-xN alloys: First-principles studies. Applied Physics Letters, 2002, vol. 80, pp. 1394-1396.

6. Davydov, V.Yu., et al. Band gap of InN and In-rich $In_xGa_{1-x}N$ alloys (0.36<x<1). Physica Status Solidi (b), 2002, vol. 230, pp. R4-R6.

7. Soshnikov, I.P., et al. Peculiarities of formation of the radiation of quantum wells. MOCVD. Fiz. Tech. Semicond., 2000, vol. 34, pp. 647-651.

8. Martinez-Criado, G., et al. Direct observation of Mn clusters in GaN by X-ray scanning microscopy. Japanese Journal of Applied Physics, 2004, vol. 43, pp. L695-L697.

9. Oestreich, M. Injecting Spin Into Electronics, Nature, www.nature.com. Macmillan Magazines Ltd, 1999, vol.402, pp.735-741.

10. Dietl, T., Ohno, H., Matsukura, F. Hole-mediated ferromagnetism in tetrahedrally coordinated semiconductors. Physical Review B, 2001, vol.63, pp. 195205.

11. Dhar, S., et al. Colossal Magnetic Moment of Gd in GaN. Physical Review Lett., 2005, vol. 94, pp. 037205.

12. Shein, I.R., et al. Magnetization of beryllium oxide in the presence of non-magnetic impurities: Boron, carbon, and nitrogen. JETP Lett., 2007, vol.85, iss. 5, pp. 246-250.

13. Baroni, S., Corso, A. Dal, de Gironcoli, S., et al. http://www.pwscf.org/.

14. Ilyasov, V.V., Zdanova, T.P., Nikiforov, I.Ya. X-ray spectra and electron energy structure of nitrogen into solid solution $Al_xGa_{1-x}N$. Fizika Tverdogo Tela, 2007, vol.49, pp.1369-1372.

15. Perdew, J.P., Burke, S., Ernzerhof, M. Generalized Gradient Approximation Made Simple. Physical Review Lett., 1996, vol. 77, p. 3865.

16. Ilyasov, V.V., Nikiforov, I.Ya., Ilyasov, Yu.V. Ti L-Spectrum XANES and electron structure of the system Ti-Al-C. Journal Physical IV France, 1997, vol.7, pp. 281-282.

17. Mecheryakov, V.F. Crystal field and the magnetization of inclined antiferromagnetic CoCO3. JETP, 2007, vol.132, pp.1138-1151.

18. Hermann, F., Skillman, S. Atomic structure calculations. Prentice-Hall, Inc., Englewood Cliffs (N.J.), 1963.

19. Ilyasov, V.V., Zdanova, T.P., Nikiforov, I.Ya. Electron energy structure and X-ray spectra of wide-gap semiconductors GaN, AlN, and AlN-GaN. Journal of Structural Chemistry, 2007, vol.48, pp.68-75.

Библиографический список

1. Nakamura, S. InGaN-based blue light-emitting diodes and laser diodes / S. Nakamura // Journal of Crystal Growth. — 1999. — Vol. 202. — P. 290-295.

2. Ferhat, M. First-principles calculations of gap bowing in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys: Relation to structural and thermodynamic properties / M. Ferhat, F. Bechstedt // Physical Review B. — 2002. — Vol. 65. — P. 075213-1 -075213-8.

3. Li, J.B., et al. Cubic InGaN grown by MOCVD / J.B. Li [et al.] // MRS Internet Journal of Nitride Semiconductor Research. — 1999. — Vol. 4S1, G3. — P. 25.

4. Krivolapchuk, V.V. The role of inserting electrical fields in the formation of the radiation of quantum wells InGaN/GaN / V.V. Krivolapchuk, V.V. Lundin, M.M. Mezdrogina // Fizika Tverdogo Tela. — 2005. — Vol. 47, № 7. — P. 1338-1342.

5. Ferhat, M. Gap bowing and Stokes shift in InxGa1-xN alloys: First-principles studies / M. Ferhat, J. Furthműller, F. Bechstedt // Applied Physics Letters. — 2002. — Vol. 80. — P. 1394-1396.

6. Davydov, V.Yu. Band gap of InN and In-rich $In_xGa_{1-x}N$ alloys (0.36<x<1) / V.Yu. Davydov [et al.] // Physica Status Solidi (b). — 2002. — Vol. 230. — P. R4-R6.

7. Soshnikov, I.P., et al. Peculiarities of formation of the radiation of quantum wells. MOCVD / I.P. Soshnikov [et al.] // Fiz. Tech. Semicond. — 2000. — Vol. 34. — P. 647-651.

8. Martinez-Criado, G. Direct observation of Mn clusters in GaN by X-ray scanning microscopy / G. Martinez-Criado [et al.] // Japanese Journal of Applied Physics. — 2004. — Vol. 43. — P. L695-L697.
9. Oestreich, M. Injecting Spin Into Electronics / M. Oestreich // Nature, Macmillan Magazines Ltd. — 1999. — Vol.402. — P.735-741.
10. Dietl, T. Hole-mediated ferromagnetism in tetrahedrally coordinated semiconductors / T. Dietl, H. Ohno, F. Matsukura // Physical Review B. — 2001. — Vol. 63. — P. 195205.
11. Dhar, S. Colossal Magnetic Moment of Gd in GaN / S. Dhar [et al.] // Physical Review Lett. — 2005. — Vol. 94. — P. 037205.
12. Shein, I.R. Magnetization of beryllium oxide in the presence of non-magnetic impurities: Boron, carbon, and nitrogen. / I.R. Shein [et al.] // JETP Lett. — 2007. — Vol. 85, iss. 5. — P. 246-250.
13. Baroni, S. Phonons and related crystal properties from density-functional perturbation theory / S. Baroni, S. de Gironcoli, A. Dal Corso, P. Giannozzi // Reviews of Modern Physics. — 2001. — Vol. 72, iss. 2. — P. 515.
14. Ilyasov, V.V. X-ray spectra and electron energy structure of nitrogen into solid solution $Al_xGa_{1-x}N$ / V.V. Ilyasov, T.P. Zdanova, T.Ya. Nikiforov // Fizika Tverdogo Tela. — 2007. — Vol.49. — P. 1369-1372.
15. Perdew, J.P. Generalized Gradient Approximation Made Simple / J.P. Perdew, S. Burke, M. Ernzerhof // Physical Review Lett. — 1996. — Vol. 77. — P. 3865.
16. Ilyasov, V.V. Ti L-Spectrum XANES and electron structure of the system Ti-Al-C / V.V. Ilyasov, I.Ya. Nikiforov, Yu.V. Ilyasov // Journal Physical IV France. — 1997. — Vol. 7. — P. 281-282.
17. Mecheryakov, V.F. Crystal field and the magnetization of inclined antiferromagnetic CoCO3 / V.F. Mecheryakov // JETP. — 2007. — Vol. 132. — P. 1138-1151.
18. Hermann, F. Atomic structure calculations / F. Hermann, S. Skillman // Prentice-Hall, Inc., Englewood Cliffs (N.J.). — 1963.
19. Ilyasov, V.V. Electron energy structure and X-ray spectra of wide-gap semiconductors GaN, AlN, and AlN-GaN / V.V. Ilyasov, T.P. Zdanova, I.Ya. Nikiforov // Journal of Structural Chemistry. — 2007. — Vol. 48. — P. 68-75.

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